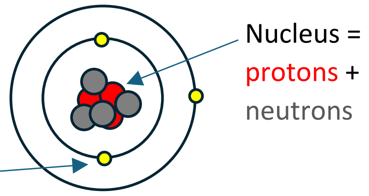
Topic 2: Atomic Structure and the Periodic Table

Students will be assessed on their ability to:

2.1 know the structure of an atom in terms of electrons, protons and neutrons

An **atom** is made up of a central nucleus containing subatomic particles called protons and neutrons, with electrons that orbit the nucleus in electron shells

Atoms are neutral as
Number of electrons = Number of protons



2.2 know the relative mass and charge of protons, neutrons and electrons

Particle	Relative mass	Relative charge
p (protons)	1	+1
n (neutrons)	1	0
e^- (electrons)	1/1840	-1

2.3 know what is meant by the terms 'atomic (proton) number' and 'mass number'

Carbon atoms

Mass number →
Atomic number →

${}^{12}_{6}C$ ${}^{13}_{6}C$

Atomic number = number of protons (= number of electrons in neutral atom)

Mass number (nucleon number) = number of protons + number of neutrons

2.4 be able to use the atomic number and the mass number to determine the number of each type of subatomic particle in an atom or ion

The **atomic** (proton) number of an atom or ion determines which element it is
The electronic configuration of an atom determines its chemical properties

2.5 understand the term 'isotope'

Isotopes are atoms of the same element that have the same number of protons but have different number of neutrons
Isotopes of the same element display the same chemical properties (as they have the same electronic configuration) but different physical properties

2.6 understand the basic principles of a mass spectrometer and be able to analyze and interpret mass spectra to:

i deduce the isotopic composition of a sample of an element

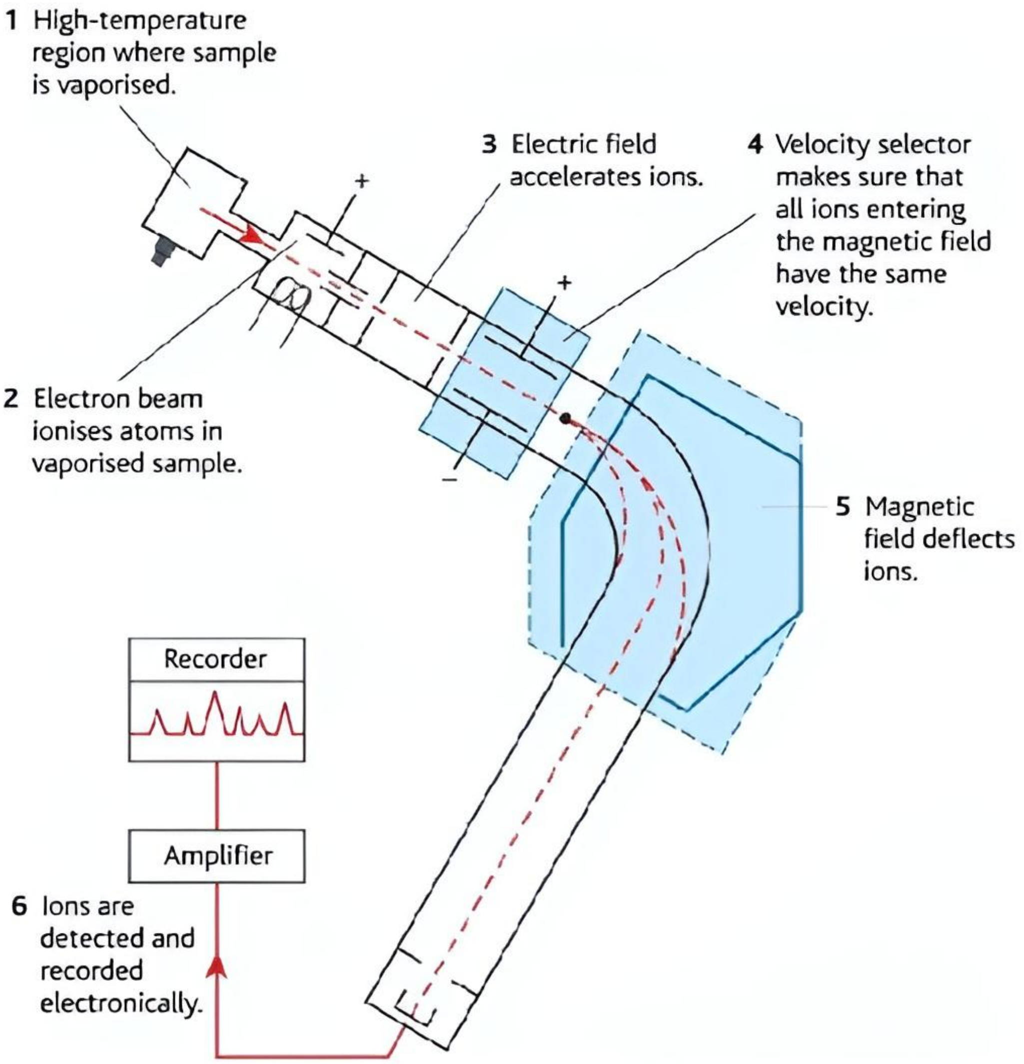
ii calculate the relative atomic mass of an element from relative abundances of isotopes and vice versa

iii determine the relative molecular mass of a molecule, and hence identify molecules in a sample

iv understand that ions in a mass spectrometer may have a 2+ charge

Isotopic composition basically means the relative abundance of different isotopes in a given sample i.e. ${}^{12}C$ ${}^{13}C$ ${}^{14}C$

$$A_r = \frac{(relative\ abundance_{isotope\ 1} \times mass_{isotope\ 1}) + (relative\ abundance_{isotope\ 2} \times mass_{isotope\ 2})\ etc}{100}$$

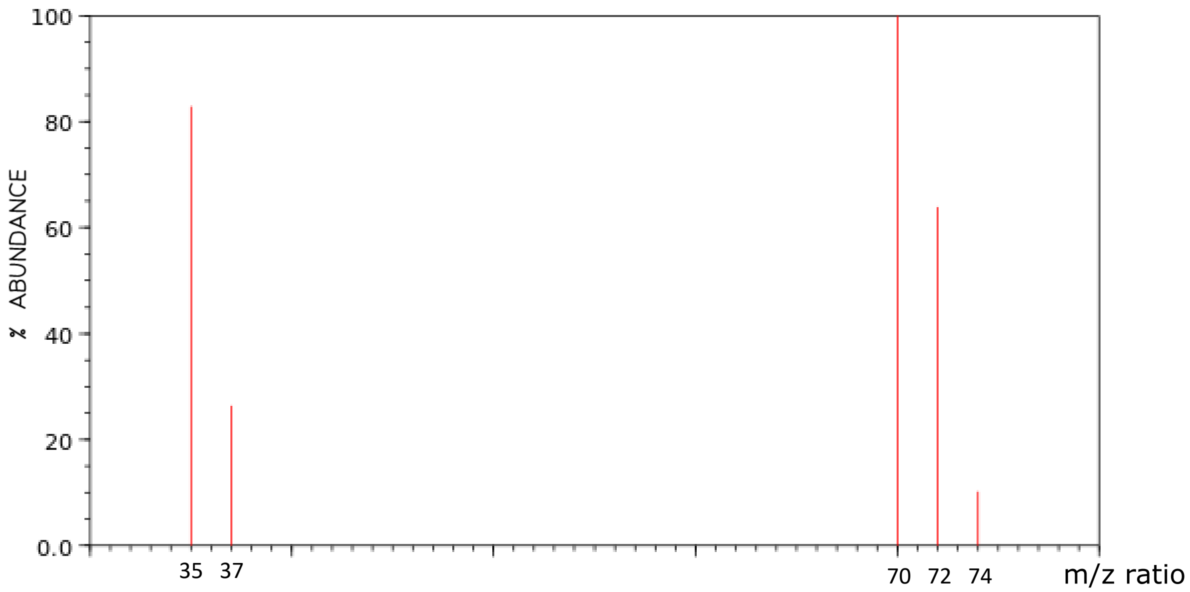


Step 1	Vaporisation	The sample is injected into a very high temperature region where it is turned into gas
Step 2	Ionisation	The gaseous sample is bombarded with high energy electrons. When the electrons hit the particles of the sample, it knocks off electrons (usually 1 electron as it does not have enough energy) and the become mostly cations with a 1+ charge
Step 3	Acceleration	The ions are accelerated by an **electric field** (not magnetic field)
Step 4	Velocity selector	The velocity selector ensures all ions entering the magnetic field have the same velocity
Step 5	Deflection	The cations are deflected by a uniform magnetic field. The amount of deflection depends on mass to charge ratio (m/z) of ions. Given that the ions have the same charge, the heavier ions will deflect less than the lighter ones. Given that the ions have the same mass, the ion with the higher charge will deflect more Only the perfect deflection will cause the path of an ion of a specific mass to bent and be detected by the mass spectrometer
Step 6	Detection	The deflected ions pass through a narrow slit and are collected on a metallic plate connected to an amplifier. For a given strength of the magnetic field, only ions with a certain m/z ratio pass through the slit and are detected

Analysing peaks!

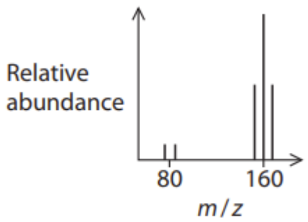
The *peak with the highest m/z value is* ***the molecular ion (M^+) peak*** whose m/z value is equal to the molecular mass (M_r) of the compound

The **[M+1] peak** is a smaller peak which is due to the natural abundance of the isotope carbon-13
The height of the [M+1] peak for a particular ion depends on how many carbon atoms are present in that molecule (this is useful in organic chem!)



2.7 be able to predict mass spectra, including relative peak heights, for diatomic molecules, including chlorine, given the isotopic abundances

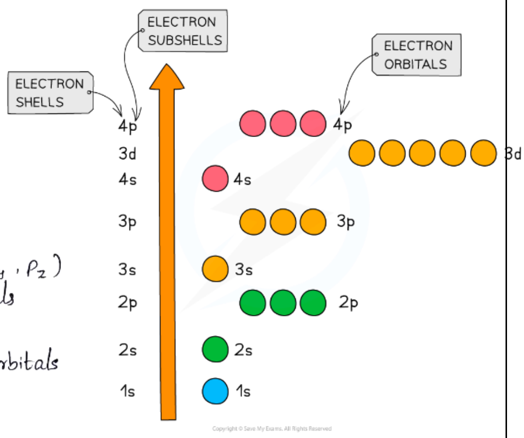
Bromine has two stable isotopes:
Br-79 and Br-81



2.8 be able to define first, second and third ionisation energies and understand that all ionisation energies are **endothermic**

Ionisation energy (IE) *is the amount of energy required to remove one mole of electrons from one mole of gaseous atoms of an element to form one mole of gaseous ions (always endothermic)*
IE is measured under standard conditions (298K & 101kPA)

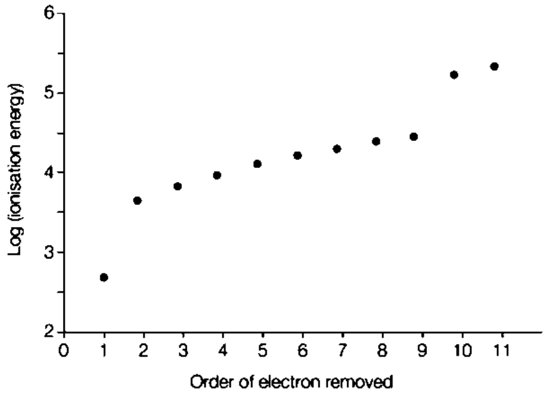
First ionisation energy:	$A(g) \rightarrow A^+(g) + e^-$
Second ionisation energy:	$A^+(g) \rightarrow A^{2+}(g) + e^-$
Third ionisation energy:	$A^{2+}(g) \rightarrow A^{3+}(g) + e^-$

2.9	know that **an orbital is a region within an atom that can hold up to two electrons with opposite spins**
	Quantum Shell > Sub-shell > Orbitals Orbitals exist at specific energy levels and electrons can only be found at these specific levels, not in between them **3** How many **orbitals** are there, in total, in the first three quantum shells of an atom? ☐ **A** 3 1^{st} Quantum shell: — 1s ← subshell ☐ **B** 6 2^{nd} Quantum shell — 2s 2p ☐ **C** 9 3^{rd} Quantum shell — 3s 3p 3d ☒ **D** 14 Each s subshell contains one s-orbital Each p subshell contains three p-orbitals (p_x, p_y, p_z) Each d subshell contains five d-orbitals ∴ Total = 3(1) + 2(3) + 1(5) = 14 orbitals 
2.10	understand how ionisation energies are influenced by the number of protons in the nucleus, the electron shielding and the sub-shell from which the electron is removed
	Ionisation energies show periodicity - a trend across a period of the Periodic Table **1. Number of protons in the nucleus** (or size of nuclear charge) The more protons there are in the nucleus, the more positively charged the nucleus is, and the more strongly electrons are attracted to it **2. Electron shielding** (from inner electrons) As the number of shells between the valence electron and positive nucleus increases, the shielding increases (shielding from both within an orbit and from inner electrons) **3. Distance of outer electrons from nucleus** The larger the size of the atom, the further the outer electrons are from the nucleus and the weaker the attraction to the nucleus

2.11 know that ideas about electronic structure developed from:

i an understanding that *successive ionisation energies provide evidence for the existence of quantum shells* and the group to which the element belongs

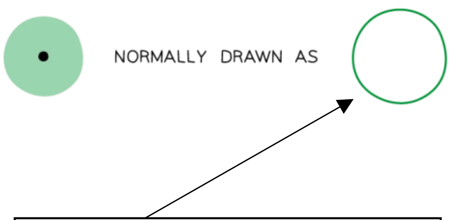
ii an understanding that *the first ionisation energy of successive elements provides evidence for electron sub-shells*



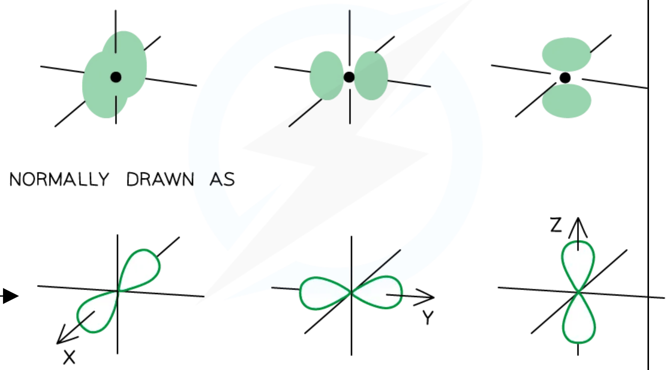
▲ **fig A** Graph showing the trend in successive ionisation energies for sodium.

The first electron being removed is on the outermost shell, furthest from the nucleus, so the first IE is the lowest
There is a big jump between the 1st and 2nd IE as the second electron being removed is from a different Quantum shell that is closer to the nucleus
There is a steady rise in ionization energy for the next 7 electrons as the electrons being removed are becoming closer to the nucleus.
There is a big jump between the 9th and 10th IE indicating that there is a change in Quantum shell
The last two electrons being removed are from the first quantum shell of lowest energy and is closest to the nucleus. Hence, the ionization energy is the highest

2.12 be able to describe the shapes of *s* and *p* orbitals



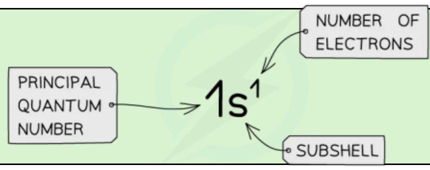
s-orbitals are spherical shaped
p-orbitals are dumbbell shaped



2.13 know that orbitals in sub-shells:

i each take a single electron before pairing up

ii pair up with two electrons of opposite spin

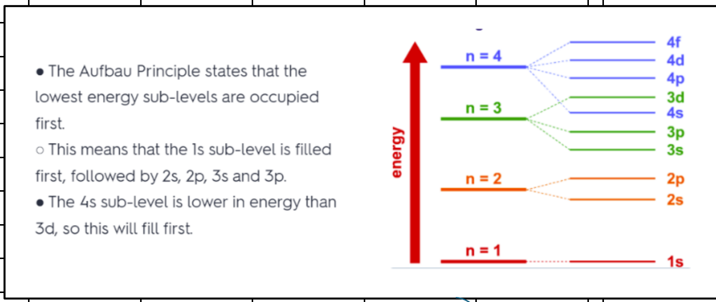


Electrons can be imagined as small spinning charges which rotate around their own axis in either a clockwise or anti-clock wise direction
Electrons with the same spin repel each other which is also called spin-pair repulsion

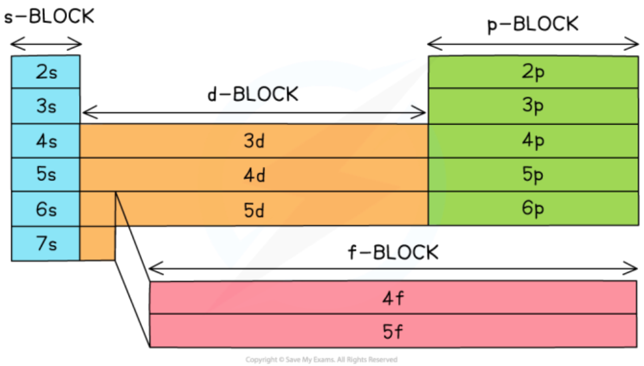
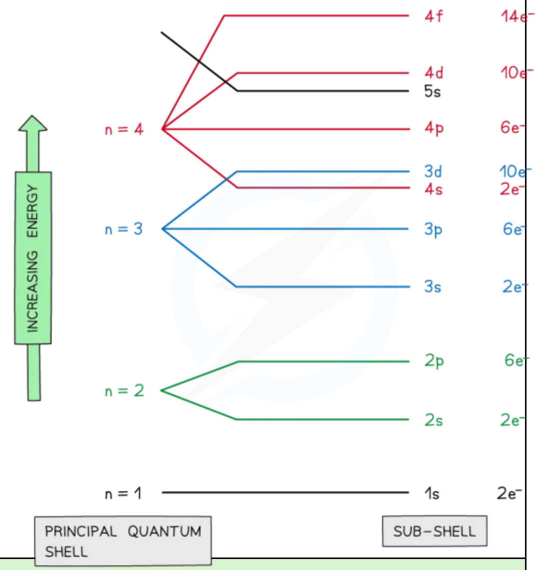
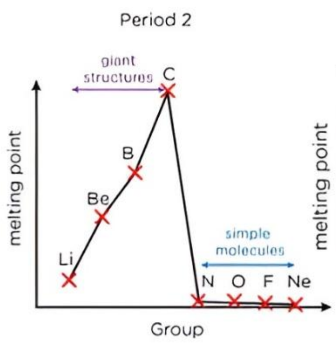
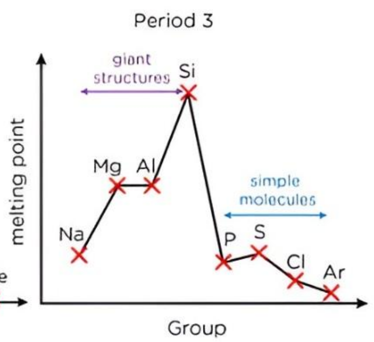
- That is why electrons will first occupy separate orbitals singly before pairing up to minimize their repulsion (this is known as Hund's rule)
- They will then pair up with its spin in the opposite direction (as Pauli Exclusion Principle states that two electrons cannot occupy the same orbital unless they have opposite spins)

2.14	be able to predict the electronic configuration of atoms of the elements from hydrogen to krypton inclusive and their ions, using *s, p, d* notation and electron-in-boxes notation

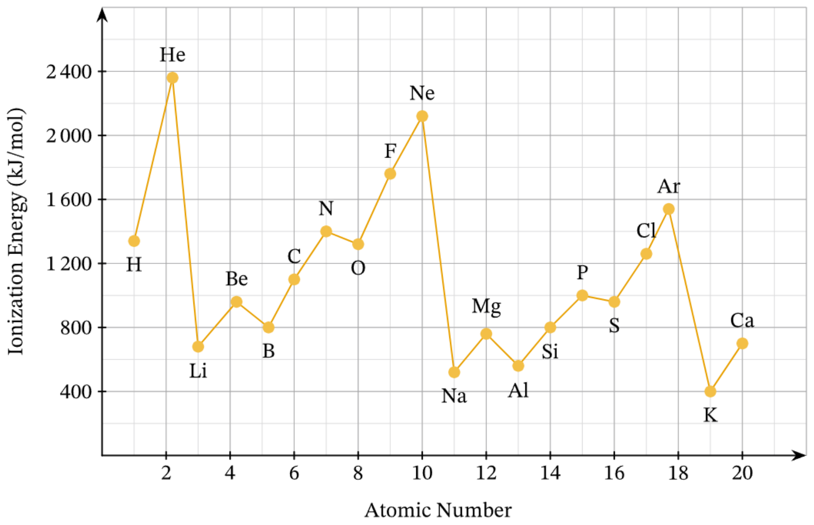
Atomic Number	Symbol	1s	2s	2p	3s	3p	3d	4s	4p
1	H	1							
2	He	2							
3	Li	2	1						
4	Be	2	2						
5	B	2	2	1					
6	C	2	2	2					
7	N	2	2	3					
8	O	2	2	4					
9	F	2	2	5					
10	Ne	2	2	6					
11	Na	2	2	6	1				
12	Mg	2	2	6	2				
13	Al	2	2	6	2	1			
14	Si	2	2	6	2	2			
15	P	2	2	6	2	3			
16	S	2	2	6	2	4			
17	Cl	2	2	6	2	5			
18	Ar	2	2	6	2	6			
19	K	2	2	6	2	6		1	
20	Ca	2	2	6	2	6		2	
21	Sc	2	2	6	2	6	1	2	
22	Ti	2	2	6	2	6	2	2	
23	V	2	2	6	2	6	3	2	
24	Cr	2	2	6	2	6	5	1	
25	Mn	2	2	6	2	6	5	2	
26	Fe	2	2	6	2	6	6	2	
27	Co	2	2	6	2	6	7	2	
28	Ni	2	2	6	2	6	8	2	
29	Cu	2	2	6	2	6	10	1	
30	Zn	2	2	6	2	6	10	2	
31	Ga	2	2	6	2	6	10	2	1
32	Ge	2	2	6	2	6	10	2	2
33	As	2	2	6	2	6	10	2	3
34	Se	2	2	6	2	6	10	2	4
35	Br	2	2	6	2	6	10	2	5
36	Kr	2	2	6	2	6	10	2	6



2.15	understand that electronic configuration determines the chemical properties of an element
	The electronic configuration of an element determines the chemical properties of that element

2.16	know that the Periodic Table is divided into blocks, such as *s, p* and *d,* and know the number of electrons that can occupy *s, p* and *d* sub-shells in the first four quantum shells
	  The subshells increase in energy as follows: s < p< d< f All the orbitals in the same subshell have the same energy and are said to be degenerate
2.17	be able to represent data, in a graphical form (including the use of logarithms of first ionisation energies on a graph) for elements 1 to 36 and hence explain the meaning of the term 'periodic property'
	Logarithms of IE is used to plot graphs as the range of values for ionization energy is too large to fit on a graph Logs make it easier to plot the values Periodic property, also called Periodicity is the repeating patterns across a period
2.18	be able to explain: i the trends in melting and boiling temperatures of the elements of Periods 2 and 3 of the Periodic Table in terms of the structure of the element and the bonding between its atoms or molecules ii the general increase and the specific trends in ionisation energy of the elements across Periods 2 and 3 of the Periodic Table iii the decrease in first ionisation energy down a group
i	  In general, as we go across both period 2 and 3, the m.pt and b.pt of both increase up to Silicon in period 3 and Carbon in period 2 After that, both m.pt and b.pt significantly decrease This is because the elements that come after silicon and carbon have simple molecular structures which only have weak intermolecular forces between its molecules

Ionization energies of the first 20 elements in the periodic table



ii

As we move across a period,

- The nuclear charge increases as the no. of protons increases
- This causes the atomic radius to decrease as outermost shell is pulled closer to the nucleus
- The shielding by inner electrons remain fairly constant as new electrons are being added to the same shell
- It becomes harder to remove an electron as there is greater attraction between the nucleus and the electron; more energy is needed

Hence, ionisation energy generally increases across a period

<u>Specific trends in period 2:</u>

Q: Why is there a slight decrease in IE between Be and B?

As Be = $1s^2\ 2s^2$ and B = $1s^2\ 2s^2\ 2p_x^1$

The outermost electron in B is in a 2p subshell which is further away from the nucleus so is less strongly attracted to it

Q: Why is there a slight decrease in IE between N and O?

As N = $1s^2\ 2s^2\ 2p_x^1\ 2p_x^1\ 2p_x^1$ and O = $1s^2\ 2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$

This means in oxygen, the electron being removed is from a full 2p-orbital that is paired while in nitrogen, the electron being removed is from a singly occupied 2p-orbital that is unpaired

More energy is required to remove an unpaired electron than a paired electron due to the spin-pair repulsion between paired electrons so less ionisation energy is needed to remove it

<u>Specific trends in period 3:</u>

Q: Why is there a slight decrease in IE between Mg and Al?

As Mg = $1s^2\ 2s^2\ 2p^6\ 3s^2$ and Al = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p_x^1$

This means the outermost electron in Al is being removed from a 3p subshell which is further away from the nucleus so is less strongly attracted to it, 3p electrons are higher in energy and are also slightly shielded by the inner electrons

Q: Why is there a slight decrease in IE between P and S?

As P = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p_x^1\ 3p_y^1\ 3p_z^1$ and S = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p_x^2\ 3p_y^1\ 3p_z^1$

This means in phosphorus, the electron being removed is from a singly-occupied p-orbital while in sulfur, the electron being removed is paired

More energy is required to remove an unpaired electron than a paired electron as there already is repulsion between paired electrons so less ionisation energy is needed to remove it

iii

As we go down a group,

- The nuclear charge increases as the no. of protons increases
- There is increased attraction between the outermost electron and the nucleus
- This means a decrease in energy of outermost electron which results in an increase in first ionization energy

However!

- One new quantum shell is added on each occasion (of going down the group)
- This means the atomic radius increases, the distance between the nucleus and the outermost electron increases
- <u>The energy of outermost electron</u> is higher (as it is in an orbital of higher energy)

3rd quantum shell energy > 2nd quantum shell energy > 1st quantum shell energy

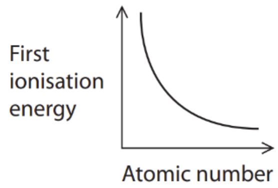
As a new quantum shell is added, the outermost electron experiences increased repulsion (shielding) from inner electrons

In summary,

effect of increase in nuclear charge < adding an extra shell + increased shielding

Hence, first ionization energy decreases down a group

!Note that first IE decrease more quickly at the start



Across a Period: Ionisation Energy Increases	Down a Group: Ionisation Energy Decreases
Increase in nuclear charge	Increase in nuclear charge
Shell number is the same Distance of outer electron to nucleus decreases	Increase in shells Distance of outer electron to nucleus increases **Shielding** effect increases, therefore, the attraction of valence electrons to the nucleus decreases
Shielding remains reasonably constant	Increased shielding
Decreased atomic/ionic radius	Increased atomic/ionic radius
The outer electron is held more tightly to the nucleus so it gets **harder** to remove it	The outer electron is held more loosely to the nucleus so it gets **easier** to remove it